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memorandum

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Tasks 2.2.7, 2.2.8, 2.2.9, 2.2.16, 2.2.17, 2.2.11, 2.2.4, 2.2.10, 2.2.12, 2.2.13 (as modified in FY18Q3), 2.2.18, and 2.2.19 were to be worked on in FY19. We also continued work on some of the older tasks, chiefly 2.2.4. The major work done in support of these tasks was as follows.

To finish up developing the second-order sensitivities of uncollided gamma rays (**task 2.2.4**), a paper submitted to *Annals of Nuclear Energy* in FY18, "Second-Order Sensitivity Analysis of Uncollided Particle Contributions to Radiation Detector Responses Using Ray-Tracing," was revised; it was accepted for publication in November 2018. Too much time was spent correcting author proofs. A paper using ray-tracing to derive previous analytic solutions was also presented at the 2018 American Nuclear Society Winter Meeting (Orlando, FL, Nov. 11–15).

Favorite overhauled the SENSMG manual. The main new feature is the subcritical multiplication and its sensitivities. There are others. It is one of the main products of this project. Favorite presented two papers on SENSMG at the 2018 American Nuclear Society Winter Meeting (Orlando, FL, Nov. 11–15). Favorite applied SENSMG to another problem important to national security and participated in a poster session at the 2018 Nuclear Explosives Code Development Conference (Los Alamos, NM, October 15–19, 2018).

In FY18, Prof. Dan Cacuci derived equations for second-order sensitivities for neutron problems, and the University of South Carolina (USC) team began implementing them in SENSMG. This work continued through FY19 and resulted in a series of three journal articles in *Energies* in which second-order sensitivities to all cross sections are given for the polyethylene-reflected BeRP ball. Most of their time in FY19 was devoted to these papers. Cacuci published a standalone article in *Annals of Nuclear Energy*, "Second-Order Adjoint Sensitivity Analysis of Ratios of Functionals of the Forward and Adjoint Fluxes in a Multiplying Nuclear System with Source."

The USC team requested nuclear data from RSICC but RSICC was unresponsive. Cacuci reported that he had inquired about the status four times and received no reply. They advanced with hypothesized covariances.

Cacuci submitted a paper on applying the second-order sensitivities to predictive modeling, "2nd-BERRU-PM: An Efficient Second-Order Predictive Modeling Methodology for Computing Best-Estimate Results with Reduced Uncertainties for Large-Scale Systems," to *Nuclear Science and Engineering*. He withdrew it from that journal but it we count it as a deliverable report for **task 2.2.13** (as modified in FY18Q3).

The second-order BERRU code was not implemented, though that was a deliverable in the USC subcontract. Second-order sensitivities of responses with respect to interface locations were not derived, though that was a deliverable in Cacuci's subcontract. There are extenuating circumstances (in particular, the mathematical difficulty of the latter), but the failure to satisfy these deliverables has been disappointing.

As of January 2020, the team at U. South Carolina continues to work on this project with their own funding. They are planning a fourth article in *Energies* that deals with second derivatives with respect to parameters of the spontaneous fission model in SOURCES4C. They fixed a long-standing bug in SOURCES4C that led to negative spontaneous fission neutron source rates in some groups. The fix was simply to increase the number of digits in SOURCES4C's value of π.

Favorite travelled to Portland, Oregon, to present a paper at the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2019; Portland, Oregon, August 25–29, 2019). The paper was "Second Derivative of an (α,n) Neutron Source with Respect to Constituent Isotope Densities."

The ANS Nonproliferation Topical meeting that was supposed to be in Wilmington, NC, in September 2018 was made into an embedded topical at the 2018 American Nuclear Society Winter Meeting (Orlando, FL, Nov. 11–15). Favorite presented an invited paper there, "On the Application of the Discrete Ordinates Method to Fixed-Source Problems (Forward and Adjoint)." This work presented the idea of using adjoint-based responses to diagnose convergence of transport solutions.

LANL post-doc Garrett Dean distributed a report, "(U) Full Monte Carlo Method for Determining Parameter Distributions in an Inverse Problem," LA-UR-18-22089, Nov. 7, 2018. This work supports tasks **2.2.7**, **2.2.8**, and **2.2.9**.

Three deliverables due in October 2018 dealt with the PM_CMPS part of the project: Distribute reports on the application of PM_CMPS for neutron leakages, neutron multiplicity, and neutron multiplication to problems with unknown interface locations. These deliverables were almost all satisfied with a conference paper, "Applying a Predictive Modeling Methodology to a Radiation Transport Inverse Problem," presented at the Radiation Protection and Shielding Topical meeting of the American Nuclear Society (Santa Fe, Aug. 26-31, 2018). This work supports tasks **2.2.7**, **2.2.8**, and **2.2.9**.

Dean made several improvements to INVERSE, the most notable being the modification to use the updated version of SOURCES4C. He began creation of a program to automate the search for a demonstration case involving unscattered gamma rays where higher-order sensitivities make a significant contribution. He also worked on confirming the equations for second-order sensitivity analysis for the first three response moments. This work supports task **2.2.10**.

Dean verified the traditional second-order sensitivity equations and determined the assumptions that go into creating them. An expansion on traditional second-order uncertainty analysis has also been completed. In it, the combined contributions from parameters are used along with the individual parameter contributions of traditional second-order uncertainty analysis. The number of terms and computations are increased, but the accuracy in predicting response moments is as well. This work supports task **2.2.10**.

This was an unexpected foray into the basics of second-order sensitivity and uncertainty analyses. We thought that the equations were well understood, even if they are rarely used. That turned out to be untrue.

A brute-force stochastic sampling algorithm was created to identify problems where the moments from the second-order uncertainty analysis differed from the first-order uncertainty analysis. A number of cases were identified in this manner with one being selected for further analysis. Response distributions were created by sampling from the input parameters using a Gaussian distribution and traditional statistical methods were used to determine the actual response moments. These were compared to the predicted moments using first-, second-, and expanded second-order uncertainty analysis. None provided an exact match to the response moments, but the more terms used in the analysis, the better the approximation was.

Dean found a test problem that demonstrated a marked improvement in using second-order uncertainty analysis over first-order uncertainty analysis. The response is the leakage of uncollided gamma rays, and the problem was highly attenuating. Using second derivatives produced an improved estimate of the response distribution moments. He documented these conclusions in a report, "Second-Order Sensitivity Analysis Equations with Uncorrelated, Independent Parameters." This work supports task **2.2.10**.

Garrett left LANL at the end of August 2019.

LANL student intern Alex Clark distributed a report, "(U) Sensitivity Analysis and Uncertainty Quantification Applied to the Feynman Y and Sm_2," LA-UR-18-30511, Oct. 29, 2018. He presented a related paper, "Sensitivity Analysis and Uncertainty Quantification of the Feynman Y and Sm_2," at the 2018 American Nuclear Society Winter Meeting, Orlando, FL, Nov. 11–15.

We have verified the adjoint-based Feynman Y sensitivity calculations in SENSMG. We did an analytic test problem, documented in "(U) Analytic One-Group S_2 Slab Problem with Isotropic Scattering and Fission Applied to Neutron Multiplicity Sensitivity," LA–UR–19–24544. We have also done a lot of central differences that are for now unpublished. A four-page summary on this work was presented at the 2019 American Nuclear Society Winter Meeting (Washington, DC, November 17–21, 2019).

Clark applied a Kalman filter to neutron multiplicity counting (NMC) experiments to optimize nuclear cross sections. He quantified the uncertainty in measured NMC experiment responses due to uncertainty in measurement parameters (source-detector distance, detector dead time, fissile source volume, density, and composition). In collaboration with LANL mentor Favorite and North Carolina State University advisor John Mattingly, Clark submitted a manuscript, "Application of Neutron Multiplicity Counting Experiments to Optimal Cross Section Adjustments," to *Nuclear Science and Engineering*. This paper is the nucleus of his PhD dissertation. He has applied sampling-based uncertainty quantification (UQ) to simulations of neutron multiplicity counting (NMC) of the BeRP ball in bare and polyethylene-reflected configurations to determine if first-order UQ adequately characterizes variations in the responses due to cross section perturbations. He found that for the cross sections to which the responses are most sensitive (Pu-239 nubar and the fission and capture cross sections), a first-order estimate of the response variance agrees well with that determined by sampling-based UQ.

Clark defended is PhD dissertation at NC State in November 2019 and became a LANL post-doc in December.

A prototype version of INVERSE has been developed that can use polynomial chaos expansion (PCE) to solve inverse transport problems with passive gamma ray, neutron multiplication, neutron leakage, and neutron-induced gamma ray measurements. This prototype was placed on version control using Git system software and is available for download by LANL staff. Using this prototype, PCE-based surrogate models were tested using the DiffeRential Evolution Adaptive Metropolis (DREAM) method. Speedups obtained by PCE for passive gamma ray and neutron multiplication were reported in the previous FY. In FY19, PCE for neutron leakage and neutron-induced gamma ray measurements were tested. Speedup factors of 30 to 60 were observed for inverse problems with neutron leakage. These results are documented in the deliverable report "Project Deliverable: Polynomial Chaos Expansion for Neutron Leakage." For inverse problems with measurements of neutron-induced gamma rays, speedup factors of 34 to 631 were obtained. These results are documented in the deliverable report "Polynomial Chaos Expansion for Neutron-induced Gamma Rays." All this work supports task **2.2.16**.

Sparse grid quadrature methods were tested for reducing the computational burden of building PCE surrogates for problems with multiple unknown parameters. Over 60 sparse grid methods (contained in the ORNL code Tasmanian, which has been compiled with a prototype version of INVERSE) have been studied and tested on a variety of inverse problems in different geometries.

Methods for building an accurate PCE surrogate module with the fewest number of transport evaluations continued to be explored. In previous quarters we looked at reducing the number of transport calculations to build a surrogate model by using sparse grid quadrature sets. We built upon the previous work by exploring ways to use the sparse grids to determine the PCE expansion order necessary to build an accurate surrogate model. This expansion order is generally problem-dependent, and it can be determined by building creating higher-order models until further increase in the order no longer changes the model. To facilitate this, we have implemented Clenshaw-Curtis sparse grid quadrature sets. The nested structure of the Clenshaw-Curtis sparse grids allows us to build increasingly higher-order surrogates with smaller numbers of transport calculations than Gaussian-type quadratures. We are now implementing a method to automatically determine when the PCE order is sufficient and comparing results obtained with Clenshaw-Curtis sparse grids to those obtained with Gaussian sparse grids. This is potentially a very fruitful area for future study.

Another current area of study is an analysis of the uncertainty quantification capabilities of the DREAM method compared to first-order uncertainty analysis. To perform this study, a capability to perform first-order uncertainty quantification has been added to the differential evolution (DE) module in a prototype version of INVERSE. Numerical tests have shown the superiority of the DREAM approach for several problems. These results will be presented in an upcoming journal article.

At the 2018 American Nuclear Society Winter Meeting (Orlando, FL, Nov. 11–15), Favorite met Marco Pigni of ORNL, PI of NA-22 project OR18-Oxygen(alpha,n)-PD3Sa. An informal collaboration was begun. Favorite derived equations for the first derivatives of the (α,n) nuclear data that are used by SOURCES4C to compute (α,n) neutron source rate densities and spectra, coded the equations into SOURCES4C, did a test problem, documented the results, and distributed a report, "(U) Sensitivity of an (α,n) Neutron Source to Nuclear Data," LA-UR-18-31273, Nov. 30, 2018. Favorite presented a paper on this topic at the 2019 American Nuclear Society Annual Meeting (Minneapolis, Minnesota, June 9–13, 2019). Favorite revised and extended the LANL report and conference paper and submitted it as a manuscript to *Annals of Nuclear Energy*. It was revised in FY20Q1 and published in December. (Too much time was spent reviewing author proofs.) This work may lead to a collaboration with Pigni et al.

In April, Favorite traveled to Berkeley, California, and presented on this project at the Nuclear Security Applications Research & Development Portfolio Review (NSARD 2019).

Outlook

We were hoping to have measured data to work with. This turned out to be harder than we had anticipated. Yes, there are many datasets from past measurement campaigns. However, it is hard to find out where they are, to find out whether they are suitable, and to get someone to interpret them and provide the responses ("measurements" with uncertainties) for us to test with.

We are working on a final project report and a Technology Readiness Level assessment.

Publications

<u>Merit-reviewed journal articles published</u>

Jeffrey A. Favorite, "Second-Order Sensitivity Analysis of Uncollided Particle Contributions to Radiation Detector Responses Using Ray-Tracing," *Annals of Nuclear Energy*, **127**, 490–501 (2019); https://doi.org/10.1016/j.anucene.2018.11.028. (LA-UR-18-24819; submitted June 26, 2018; accepted Nov.13, 2018; available on-line Jan. 24, 2019; in print May 2019.)

D. G. Cacuci, "Application of the Second-Order Comprehensive Sensitivity Analysis Methodology to Compute 1st- and 2nd-Order Sensitivities of Flux Functionals in a Multiplying System with Source," *Nuclear Science and Engineering*, **193**, *6*, 55–600 (2019); https://doi.org/10.1080/00295639.2018.1553910. (Submitted July 27, 2018; accepted Nov. 27, 2018; available on-line Feb. 26, 2019; in print June 2019.)

D. G. Cacuci, "Second-Order Sensitivities of a General Functional of the Forward and Adjoint Fluxes in a Multiplying Nuclear System with Source," *Nuclear Engineering and Design*, **344**, *1*, 83–106 (2019); https://doi.org/10.1016/j.nucengdes.2019.01.007. (Submitted Aug. 14, 2018; accepted Jan. 5, 2019; available on-line Feb. 1, 2019; in print April 2019.)

D. G. Cacuci, "Second-Order Sensitivity and Uncertainty Analysis of the Roussopoulos-Functional for a Subcritical Multiplying Nuclear System with Source," *Annals of Nuclear Engineering*, **126**, 281–291 (2019); https://doi.org/10.1016/j.anucene.2018.11.022. (Submitted Aug. 21, 2018; accepted Nov. 9, 2018; available on-line Nov. 22, 2018; in print April 2019.)

D. G. Cacuci, "The Roussopoulos and Schwinger Functionals for Nuclear Systems Involving Imprecisely Known Fluxes and/or Parameters: Distinctions and Equivalences," *Nuclear Science and Engineering*, **193**, *7*, 681–721 (2019); https://doi.org/10.1080/00295639.2018.1564504. (Submitted Aug. 29, 2018; accepted Dec. 26, 2018; available on-line March 11, 2019; in print July 2019.)

D. G. Cacuci, "Alternative Adjoint Boltzmann Transport Operators In Alternative Hilbert Spaces in Spherical Geometry: Theory and Illustrative Application," *Nuclear Science and Engineering*, **193**, *9*, 927–947 (2019); https://doi.org/10.1080/00295639.2019.1582934. (Submitted April 14, 2018; accepted Feb. 12, 2019; available on-line April 8, 2019; in print September 2019.)

R. Fang and D. G. Cacuci, "Comprehensive Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) Applied to a Subcritical Experimental Reactor Physics Benchmark: II. Effects of Imprecisely Known Microscopic Scattering Cross Sections," *Energies*, **12**, *21* (2019); https://doi.org/10.3390/en12214114. (Submitted Aug. 27, 2019; accepted Oct. 23, 2019; available on-line Oct. 28, 2019; in print N/A.)

D. G. Cacuci, R. Fang, J. A. Favorite, M. C. Badea, and F. Di Rocco, "Comprehensive Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) Applied to a Subcritical Experimental Reactor Physics Benchmark: III. Effects of Imprecisely Known Microscopic Fission Cross Sections and Average Number of Neutrons per Fission," *Energies*, **12**, *21*

(2019); https://doi.org/10.3390/en12214100. (Submitted Aug. 27, 2019; accepted Oct. 21, 2019; available on-line Oct. 27, 2019; in print N/A.)

D. G. Cacuci, R. Fang, and J. A. Favorite, "Comprehensive Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) Applied to a Subcritical Experimental Reactor Physics Benchmark: I. Effects of Imprecisely Known Total and Capture Cross Sections," *Energies***12**, *21* (2019); https://doi.org/10.3390/en12214219. (Submitted Aug. 27, 2019; accepted Nov. 1, 2019; available on-line Nov. 5, 2019; in print N/A.)

Dan Gabriel Cacuci, "Second-Order Adjoint Sensitivity Analysis of a General Ratio of Functionals of the Forward and Adjoint Fluxes in a Multiplying Nuclear System with Source," *Annals of Nuclear Energy*, **135** (2020); https://doi.org/10.1016/j.anucene.2019.106956. (Submitted May 22, 2019; accepted July 24, 2019; available on-line Aug. 22, 2019; in print Jan. 2020.)

Jeffrey A. Favorite, "Sensitivity of an (α,n) Neutron Source to (α,n) Cross Sections and Stopping Powers," *Annals of Nuclear Energy*, **138** (2020); https://doi.org/10.1016/j.anucene.2019.107154. (Submitted July 22, 2019; accepted Oct. 18, 2019; available on-line Dec. 12, 2019; in print April 2020.)

<u>Merit-reviewed journal articles accepted for publication</u>

Alexander R. Clark, John Mattingly, and Jeffrey A. Favorite, "Application of Neutron Multiplicity Counting Experiments to Optimal Cross Section Adjustments," *Nuclear Science and Engineering*, to be published (2020); https://doi.org/10.1080/00295639.2019.1698267. (Submitted Sept. 9, 2019; accepted Nov. 25, 2019.)

<u>Merit-reviewed conference proceedings</u>

Jeffrey A. Favorite, "On the Application of the Discrete Ordinates Method to Fixed-Source Problems (Forward and Adjoint)," *Proceedings of the Advances in Nuclear Nonproliferation Technology and Policy Conference 2018 – (ANTPC-2018)*, CD-ROM, Orlando, Florida, November 11–15 (2018).

Keith C. Bledsoe, Matthew A. Jessee, and Douglas E. Peplow, "Uncertainty Analysis for Neutron Active Interrogation Calculations," *Proceedings of the Advances in Nuclear Nonproliferation Technology and Policy Conference 2018 – (ANTPC-2018)*, CD-ROM, Orlando, Florida, November 11–15 (2018).

Jeffrey A. Favorite, "Analytic Solutions for a Homogeneous Sphere Derived Using Ray-Tracing," *Transactions of the American Nuclear Society*, **119**, 663–666 (2018). Presented at the 2018 American Nuclear Society Winter Meeting, Orlando, Florida, November 11–15, 2018.

Jeffrey A. Favorite, "SENSMG: A New Tool for Multigroup Discrete Ordinates Sensitivity Analysis for Criticality," *Transactions of the American Nuclear Society*, **119**, 859–862 (2018). Presented at the 2018 American Nuclear Society Winter Meeting, Orlando, Florida, November 11–15, 2018.

Jeffrey A. Favorite, "SENSMG: A New Tool for Multigroup Discrete Ordinates Sensitivity Analysis for Shielding," *Transactions of the American Nuclear Society*, **119**, 1053–1056 (2018). Presented at the 2018 American Nuclear Society Winter Meeting, Orlando, Florida, November 11–15, 2018.

Alexander Clark, Jeffrey A. Favorite, Alexander McSpaden, and Mark Nelson, "Sensitivity Analysis and Uncertainty Quantification of the Feynman Y and Sm_2," *Transactions of the American Nuclear Society*, **119**, 805–808 (2018). Presented at the 2018 American Nuclear Society Winter Meeting, Orlando, Florida, November 11–15, 2018.

Jeffrey A. Favorite, "Derivative of an (α,n) Neutron Source with Respect to Nuclear Data," *Transactions of the American Nuclear Society*, **120**, 784–787 (2019). Presented at the 2019 American Nuclear Society Annual Meeting, Minneapolis, Minnesota, June 9–13, 2019.

Jeffrey A. Favorite, "Second Derivative of an (α,n) Neutron Source with Respect to Constituent Isotope Densities," *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2019)*, Portland, Oregon, August 25–29 (2019).

Jeffrey A. Favorite, "Analytic One-Group S_2 Slab Problem with Isotropic Scattering and Fission Applied to Leakage and Neutron Multiplicity Sensitivity," *Transactions of the American Nuclear Society*, **121**, 929–932 (2019). Presented at the 2019 American Nuclear Society Winter Meeting, Washington, DC, November 17–21, 2019.

Other presentations

Jeffrey A. Favorite and Cory D. Ahrens, "Adjoint-Based Neutronic Sensitivity Analysis of a Particular Underground Test," poster presented at the 2018 Nuclear Explosives Code Development Conference (NECDC), Los Alamos, New Mexico, October 15–19, 2018.

Jeffrey A. Favorite, "Predictive Modeling, Inverse Problems, and Uncertainty Quantification with Application to Emergency Response," LA–UR–19–22281, March 2019, viewgraphs and summary for the Nuclear Security Applications Research & Development Portfolio Review (NSARD 2019), Berkeley, CA, April 9–11, 2019.

Other: Internal Reports

Alex Clark, "Sensitivity Analysis and Uncertainty Quantification Applied to the Feynman Y and Sm_2," Los Alamos National Laboratory report LA-UR-18-30511, October 29, 2018.

Jeffrey A. Favorite, "LA17-V-InverseRadTransportProblem-PD2Kb FY2018 Annual Report," Los Alamos National Laboratory report LA–UR–18–30645, November 5, 2018.

Garrett Dean, "Full Monte Carlo Method for Determining Parameter Distributions in an Inverse Problem," Los Alamos National Laboratory report LA-UR-18-22089, November 7, 2018.

Jeffrey A. Favorite, "Sensitivity of an (α,n) Neutron Source to Nuclear Data," Los Alamos National Laboratory report LA-UR-18-31273, November 30.

Keith C. Bledsoe and Matthew A. Jessee, "Project Deliverable: Polynomial Chaos Expansion for Neutron Leakage (LA17-V-InverseRadTransportProblem-PD2Kb)," Oak Ridge National Laboratory report ORNL/SPR-2018/1073 (December 2018).

Jeffrey A. Favorite, "(U) PARTISN Feature Request: Unnormalized Chi Vector," Los Alamos National Laboratory report XCP-3:19–008(U), March 11, 2019.

Jeffrey A. Favorite, "(U) Analytic One-Group S_2 Slab Problem with Isotropic Scattering and Fission Applied to Neutron Multiplicity Sensitivity," Los Alamos National Laboratory report LA–UR–19–24544, May 16, 2019; Rev. 1, May 22, 2019.

Dan Gabriel Cacuci, "2nd-BERRU-PM: An Efficient Second-Order Predictive Modeling Methodology for Computing Best-Estimate Results with Reduced Uncertainties for Large-Scale Systems," May 27, 2019.

Jeffrey A. Favorite, "(U) SENSMG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff}, α, and Subcritical Multiplication Using PARTISN," Los Alamos National Laboratory report LA–UR–19–26249, Rev. 0, July 1, 2019; Rev.1, September 19, 2019.

Garrett Dean, "Second-Order Sensitivity Analysis Equations with Uncorrelated, Independent Parameters," Los Alamos National Laboratory report, August 26, 2019.

Keith C. Bledsoe, Jordan P. Lefebvre, and Matthew A. Jessee, "Project Deliverable: Polynomial Chaos Expansion for Neutron-Induced Gamma (LA17-V-InverseRadTransportProblem-PD2Kb)," Oak Ridge National Laboratory report ORNL/SPR-2019/1283 (September 2019).

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